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Notice of Allowance: March 8, 2004  
Application No.: 09/629,557

Our Ref. No. 4239-55412  
First Named Inventor: Miller et al.  
For: METHODS FOR PREDICTING THE BIOLOGICAL,  
CHEMICAL AND PHYSICAL PROPERTIES OF  
MOLECULES FROM THEIR SPECTRAL PROPERTIES  
Confirmation No. 4093  
Filed: July 31, 2000

Replacement Sheet (Sheet 1 of 31)

SDBS- $^{13}\text{C}$ NMR SDBS No. 1716CDS-12-007

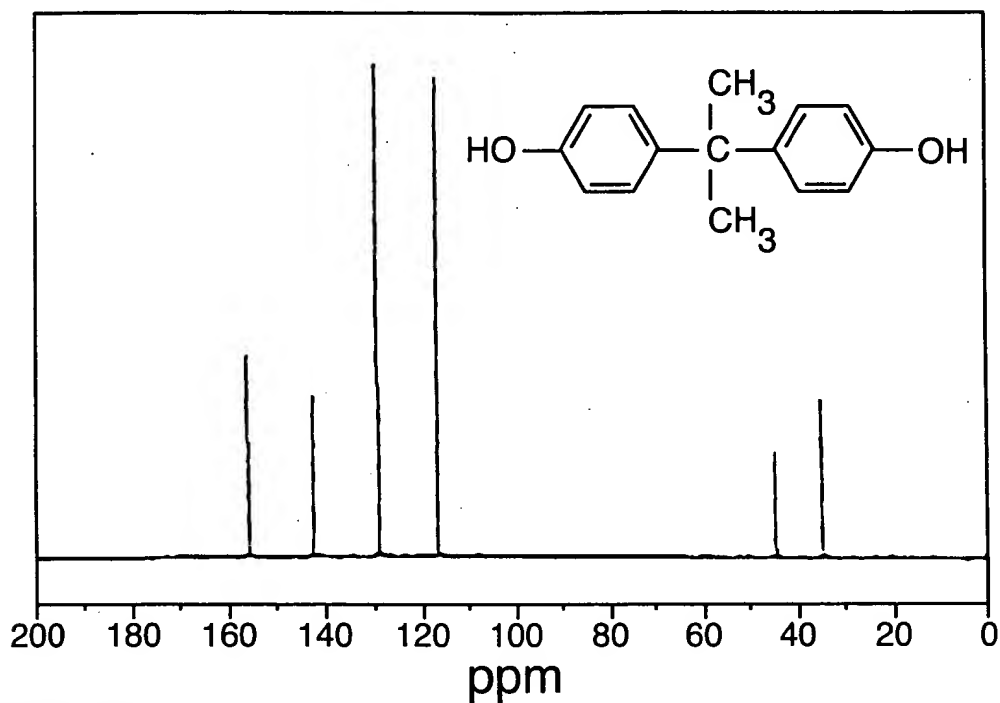
$\text{C}_{15}\text{H}_{16}\text{O}_2$

4, 4' - ISOPROPYLIDENEDIPHENOL

FIG. 1(a)

22.53 MHz

0.025 g : 0.5 ml DMSO- $\text{d}_5$



SDBS-Mass

MS-NW-6834

SDBS No. - 1716

4, 4' - ISOPROPYLIDENEDIPHENOL

(Mass of molecular ion: 228)

FIG. 1(b)

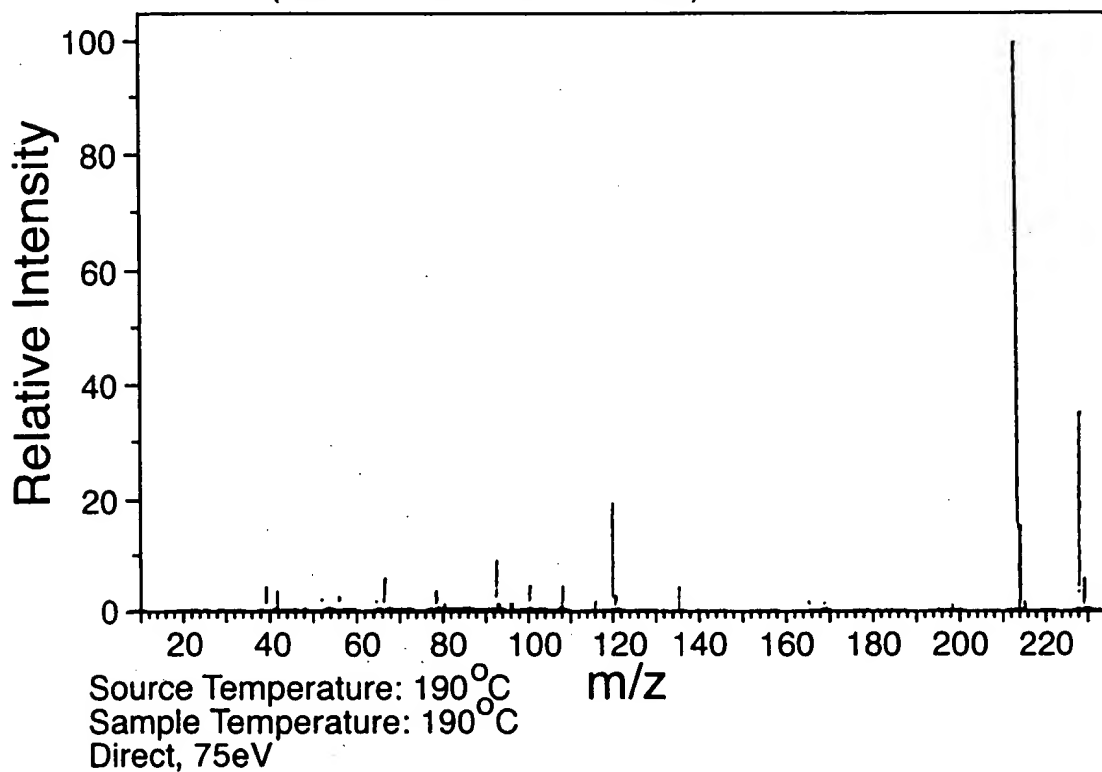
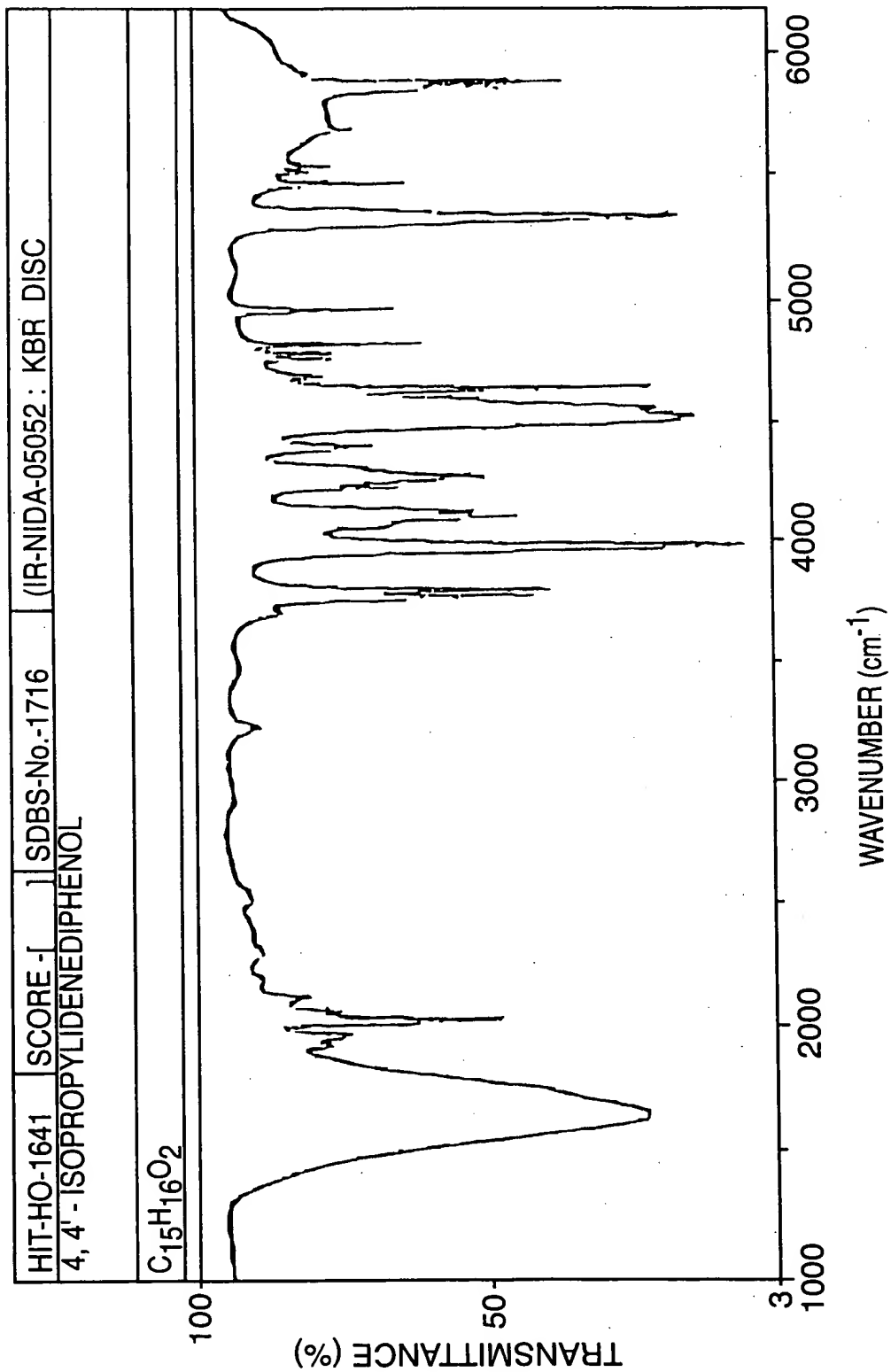


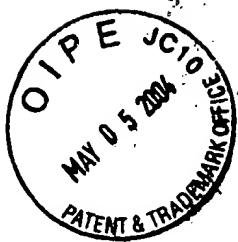
FIG. 1(c)

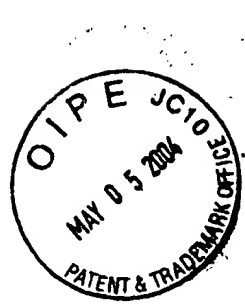


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Replacement Sheet (Sheet 2 of 31)



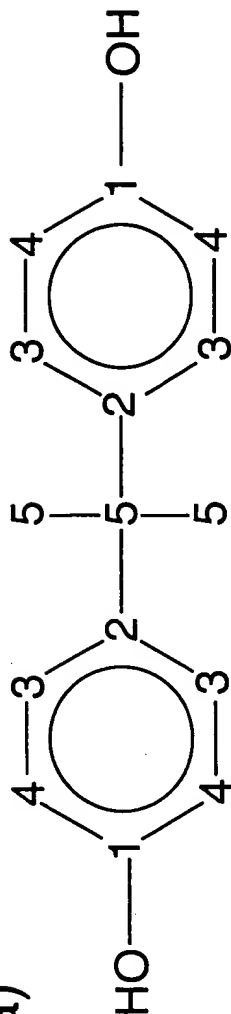


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FIG. 2(a)

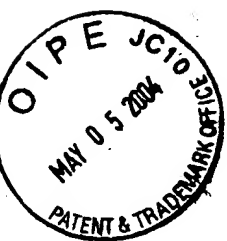


$^{13}\text{C}$	$\delta$	ppm	Int.	Assign.
1		154.72	411	
2		140.94	330	
3		127.11	1000	
4		114.43	977	
5		40.78	223	
6		30.73	328	

FIG. 2(c)

$\text{CM}^{-1} \text{ \%T CM}^{-1} \text{ \%T CM}^{-1} \text{ \%T CM}^{-1} \text{ \%T CM}^{-1} \text{ \%T CM}^{-1} \text{ \%T}$

3168 21	2933 72	1436 49	1178 20	816 66	
3070 74	2871 77	1384 62	1150 74	759 60	
3050 74	1512 39	1263 47	1113 72	755 77	
3030 70	1600 37	1295 66	1102 72	724 72	
2076 46	1510 4	1247 14	1085 57	650 58	
2966 45	1483 62	1239 12	1013 62	585 41	
2966 62	1447 42	1221 19	827 14	553 34	



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## SDBS-Mass

## FIG. 2(b)

MS-NW-6834

SDBS NO. - 1716

4, 4' - ISOPROPYLIDENEDIPHENOL

$C_{15}H_{16}O_2$

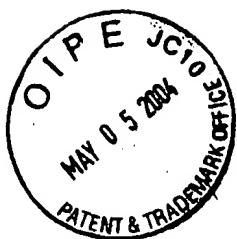
/Mass of molecular ion:

228:

m/z ratio

---

27.0	1
39.0	4
41.0	3
51.0	2
55.0	2
63.0	2
65.0	5
66.0	1
76.0	1
77.0	3
79.0	1
89.0	1
90.0	1
91.0	9
92.0	1
94.0	2
95.0	1
99.0	4
105.0	1
106.5	2
107.0	4
114.0	1
115.0	1
119.0	19
120.0	2
134.0	1
135.0	4
152.0	1
165.0	2
169.0	1
181.0	1
183.0	1
195.0	1
197.0	1
198.0	1
212.0	1
213.0	100
214.0	15
215.0	1
229.0	35
239.0	5



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Bin Number	Spectral Intensity	Bin Number	Spectral Intensity	Bin Number	Spectral Intensity
51	2	183	1	1025	62
55	2	195	1	1026	42
63	2	197	1	1027	49
65	5	198	1	1032	62
66	1	212	1	1034	47
76	1	213	100	1041	66
77	3	214	15	1046	14
79	1	215	1	1047	12
89	1	228	35	1048	19
90	1	229	5	1053	20
91	9	580	328	1056	74
92	1	590	223	1059	72
94	2	664	977	1060	72
95	1	677	1000	1062	57
99	4	690	330	1069	62
105	1	704	441	1088	14
106	2	834	21	1089	55
107	4	864	74	1095	60
114	1	866	74	1097	77
115	1	868	70	1098	72
119	19	873	46	1106	68
120	2	874	46	1114	41
134	1	875	62	1115	34
135	4	877	72		
152	1	883	77		
165	2	1009	39		
169	1	1011	37		
181	1	1019	4		

**FIG. 3 – a hypothetical set of spectrally derived molecular structure descriptors for bisphenol A.**

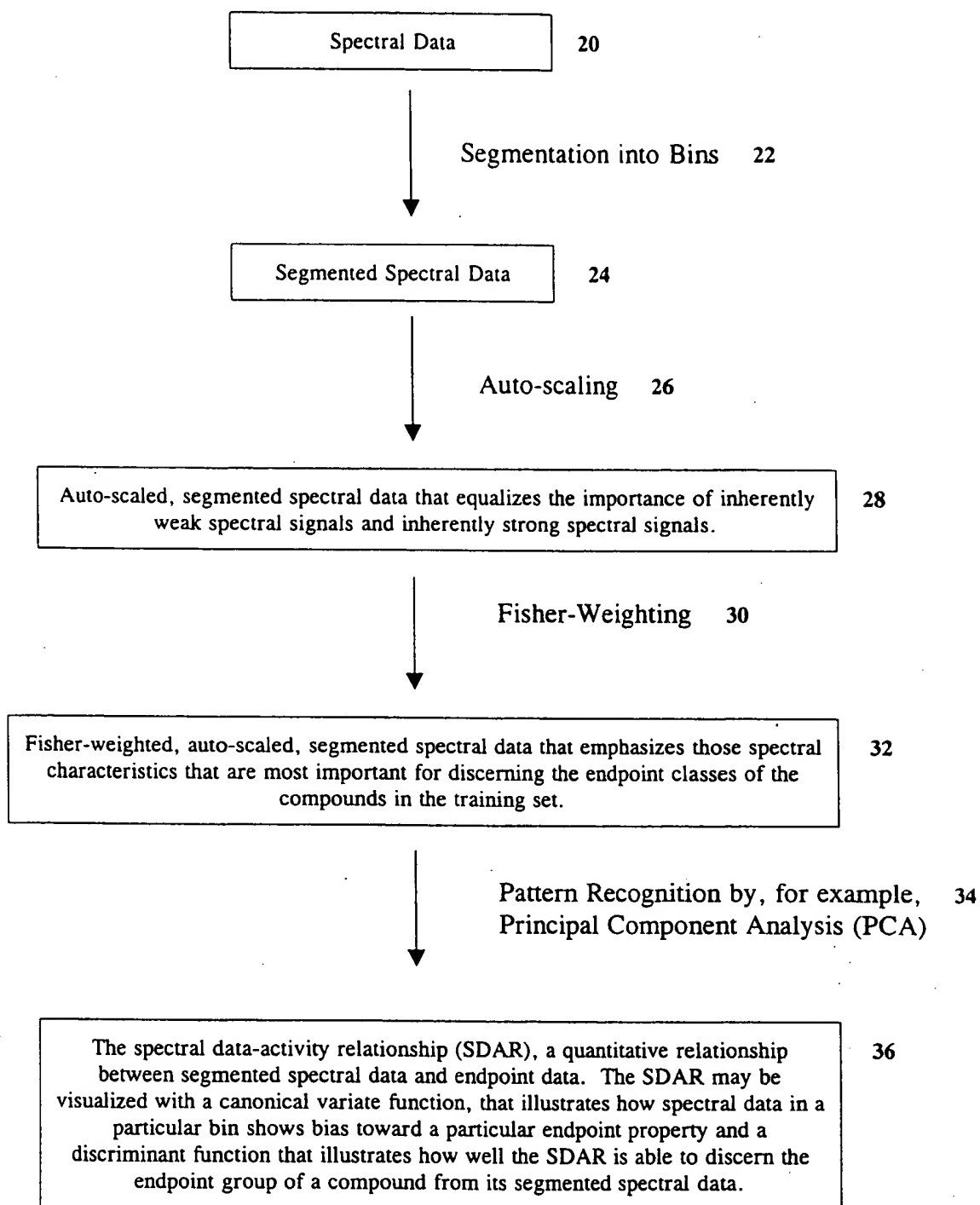
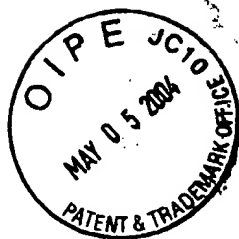


FIG. 4



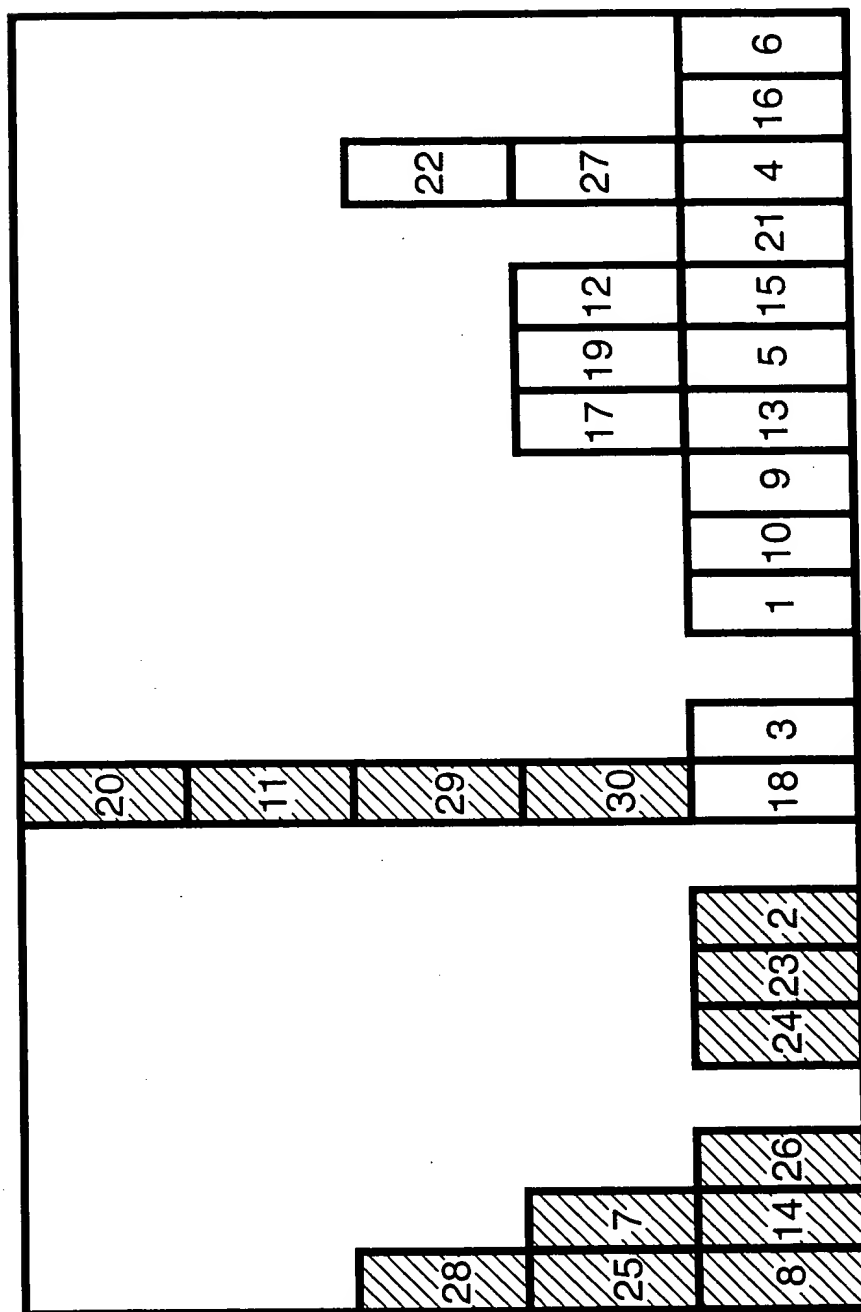
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# DISCRIMINANT FUNCTION

FIG. 5



Component 1

Component Frequency



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# CANONICAL VARIATE 1

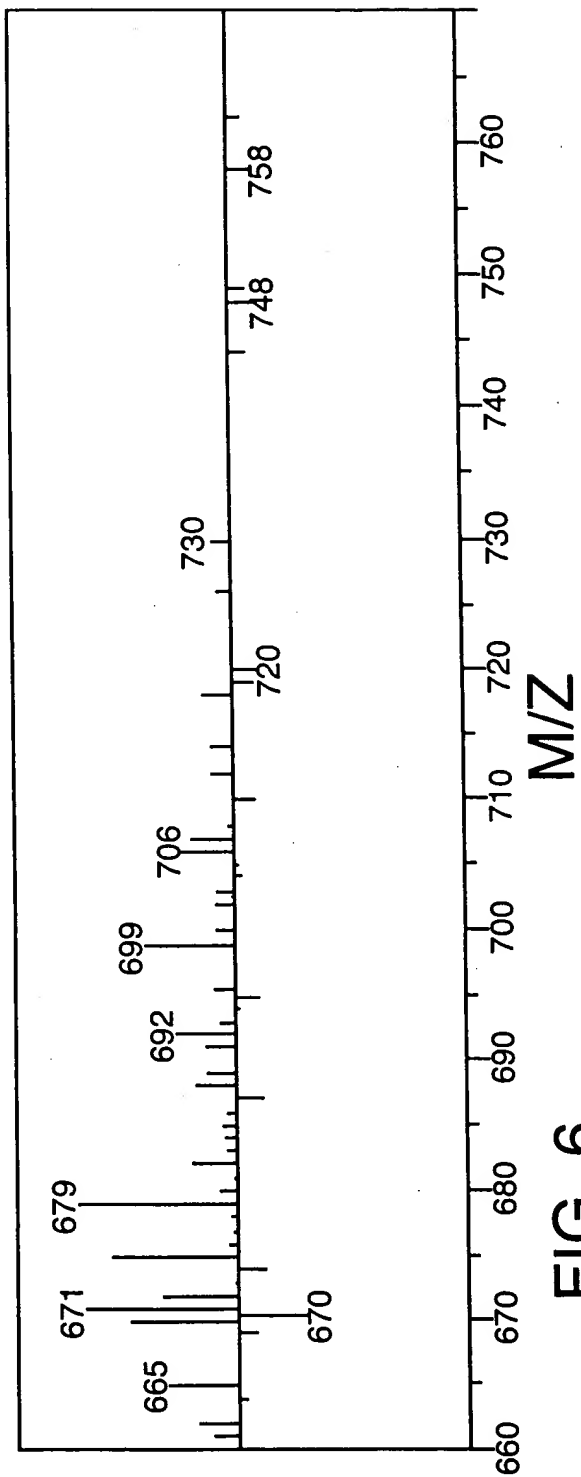
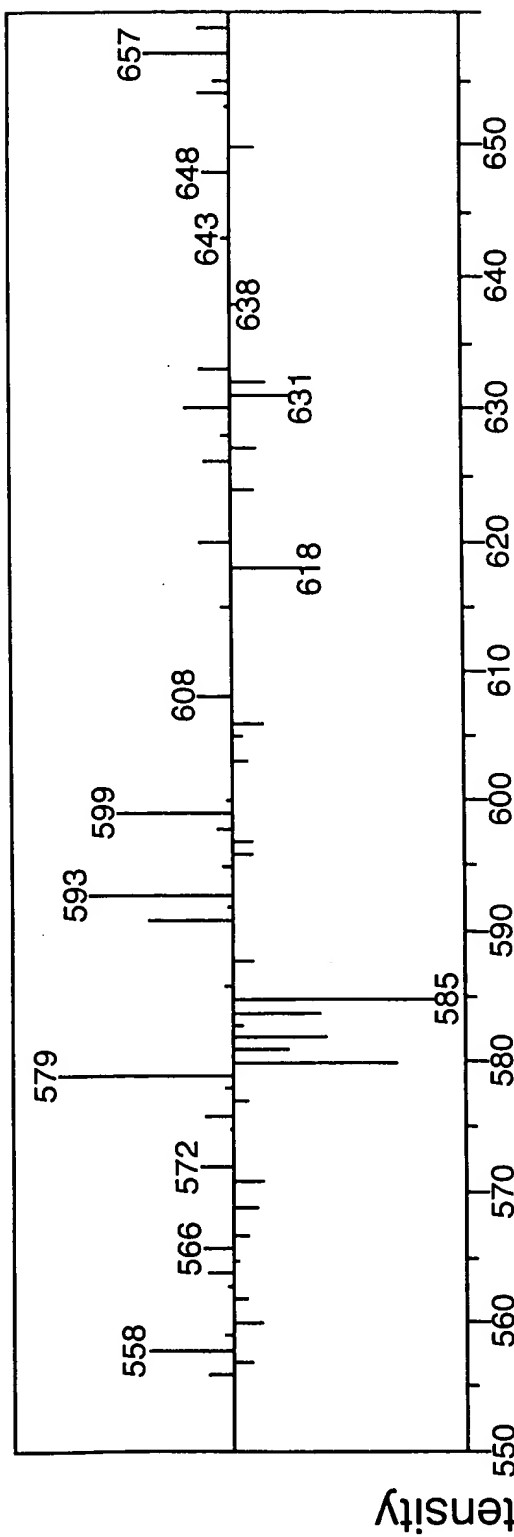
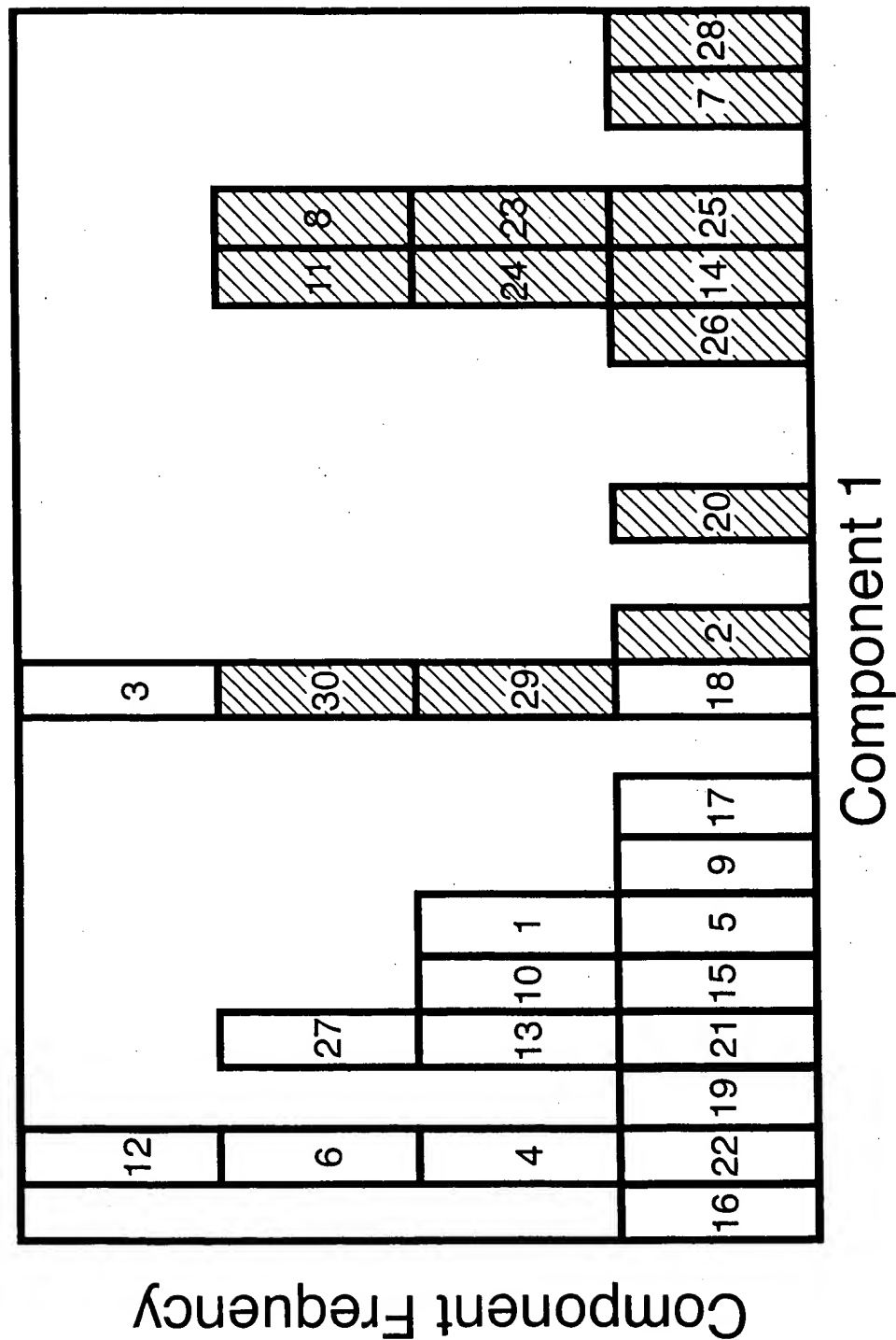


FIG. 6



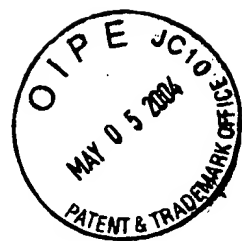
FIG. 7 DISCRIMINANT FUNCTION

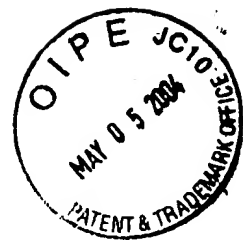


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# CANONICAL VARIATE 1

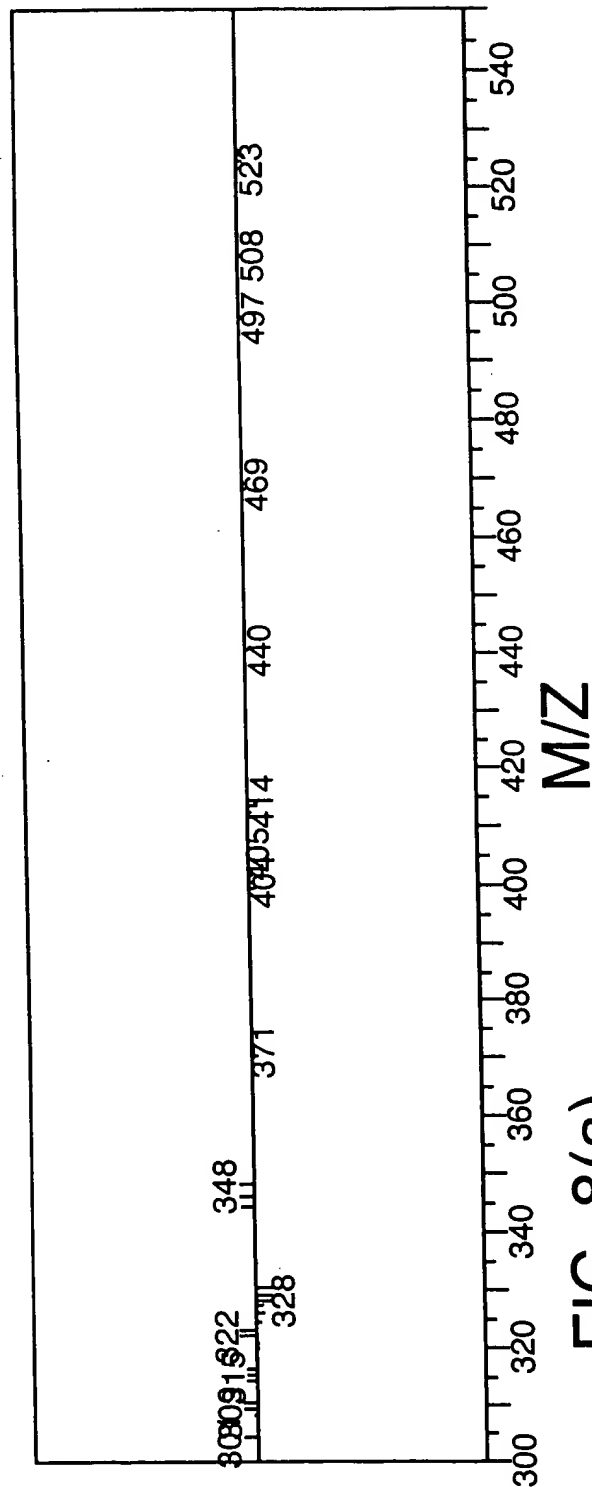
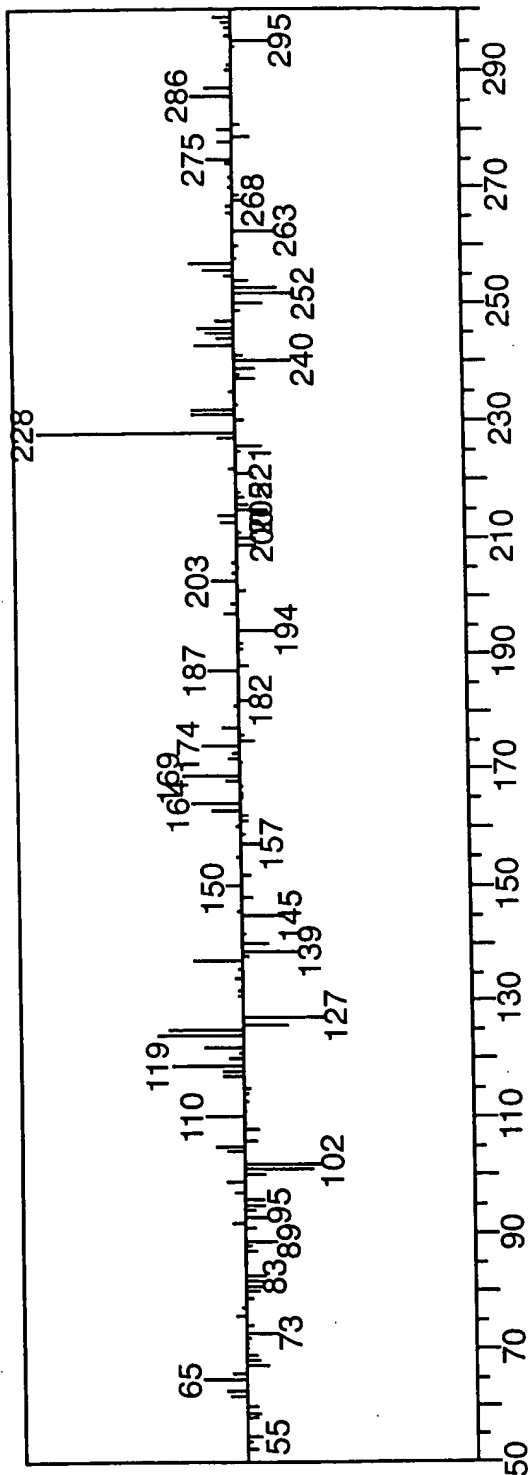


FIG. 8(a)

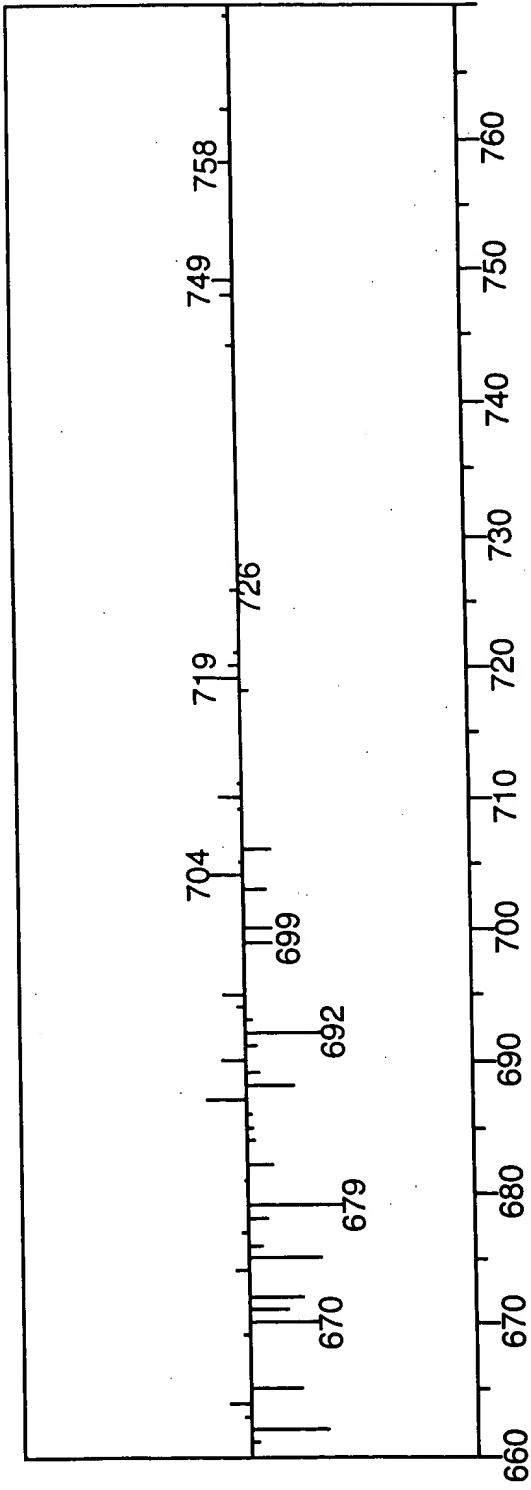
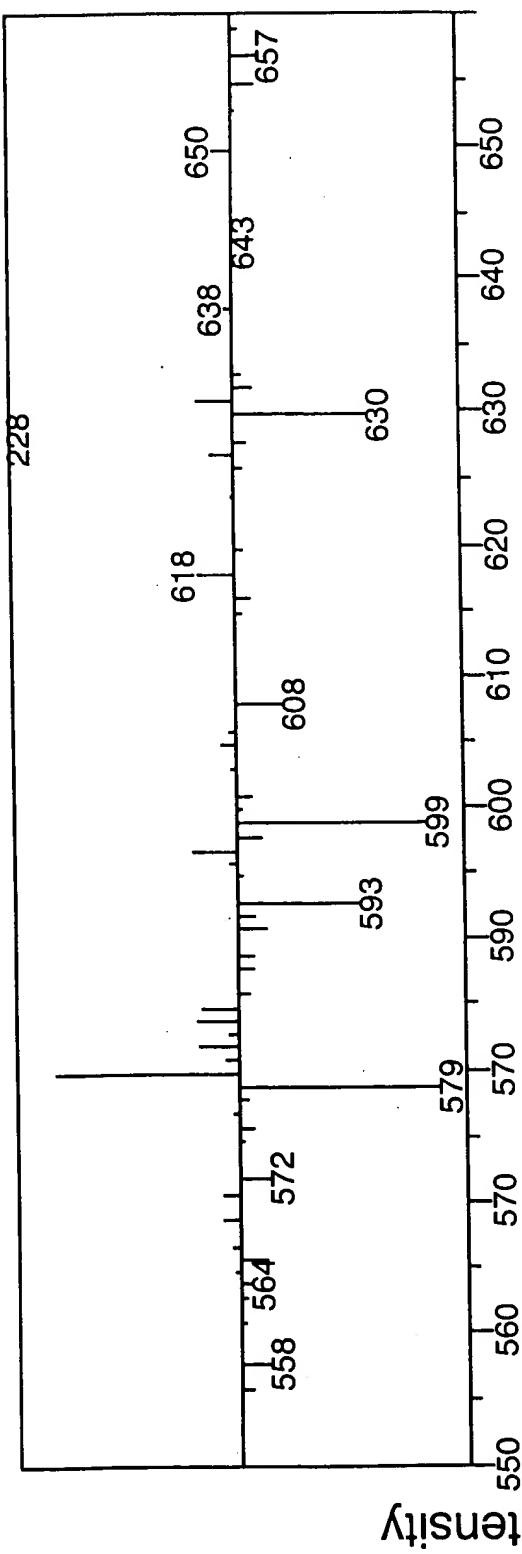


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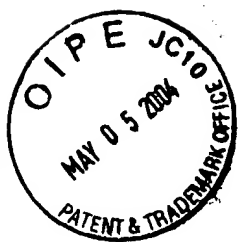
Replacement Sheet (Sheet 11 of 31)

CANONICAL VARIATE 1



M/Z

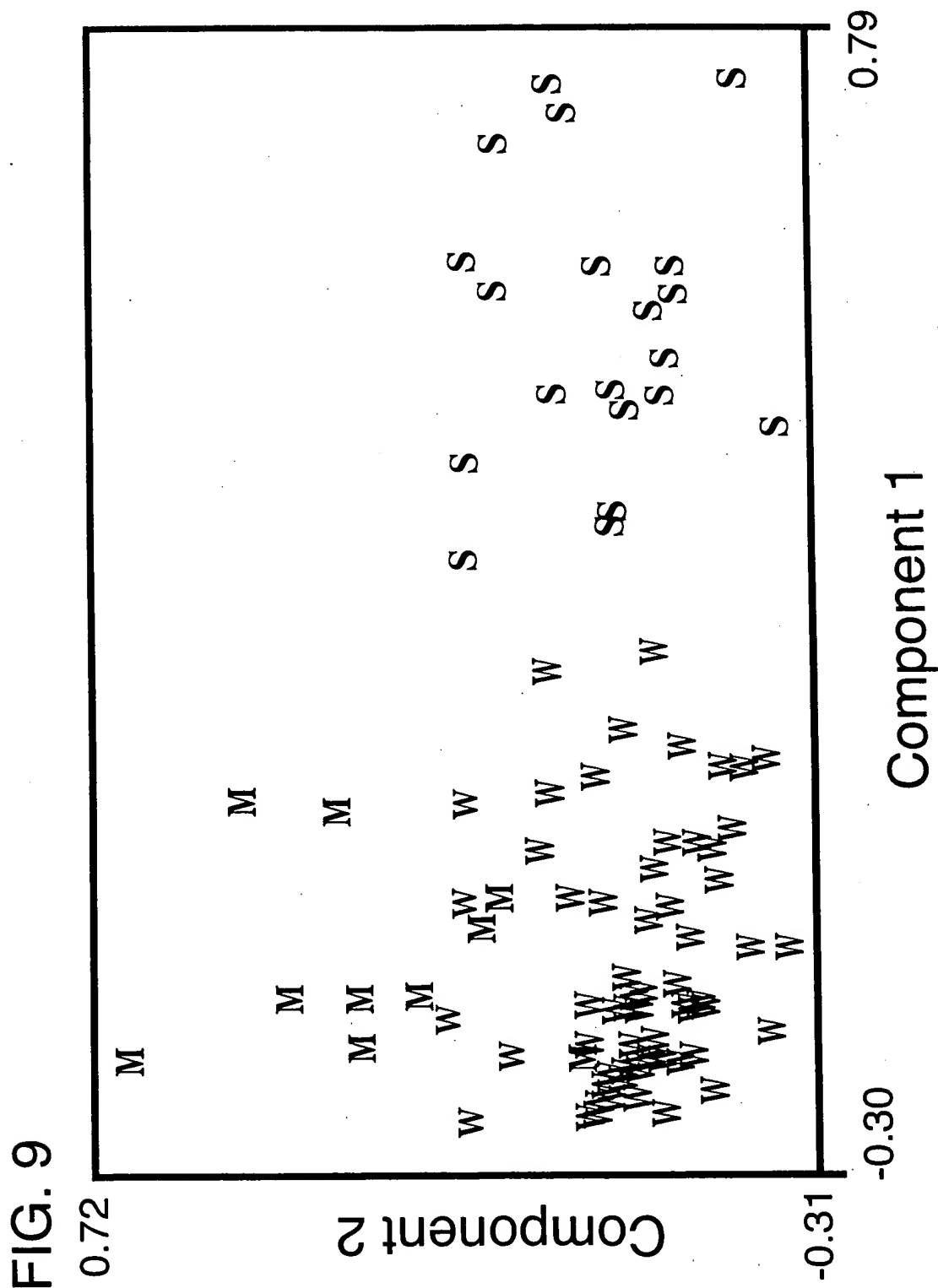
FIG. 8(b)



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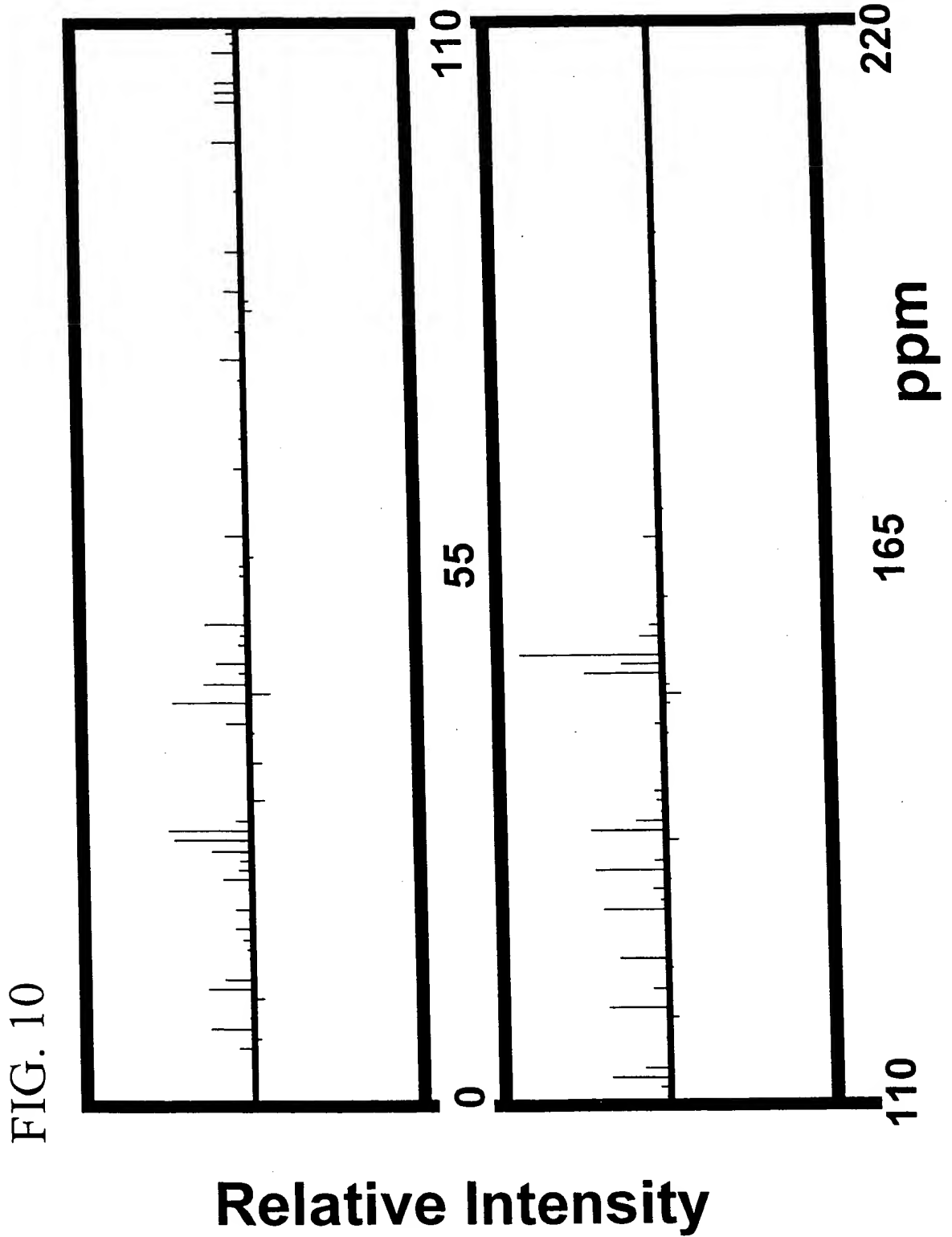


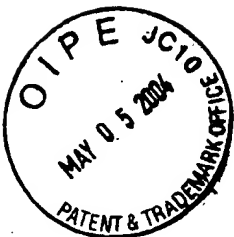


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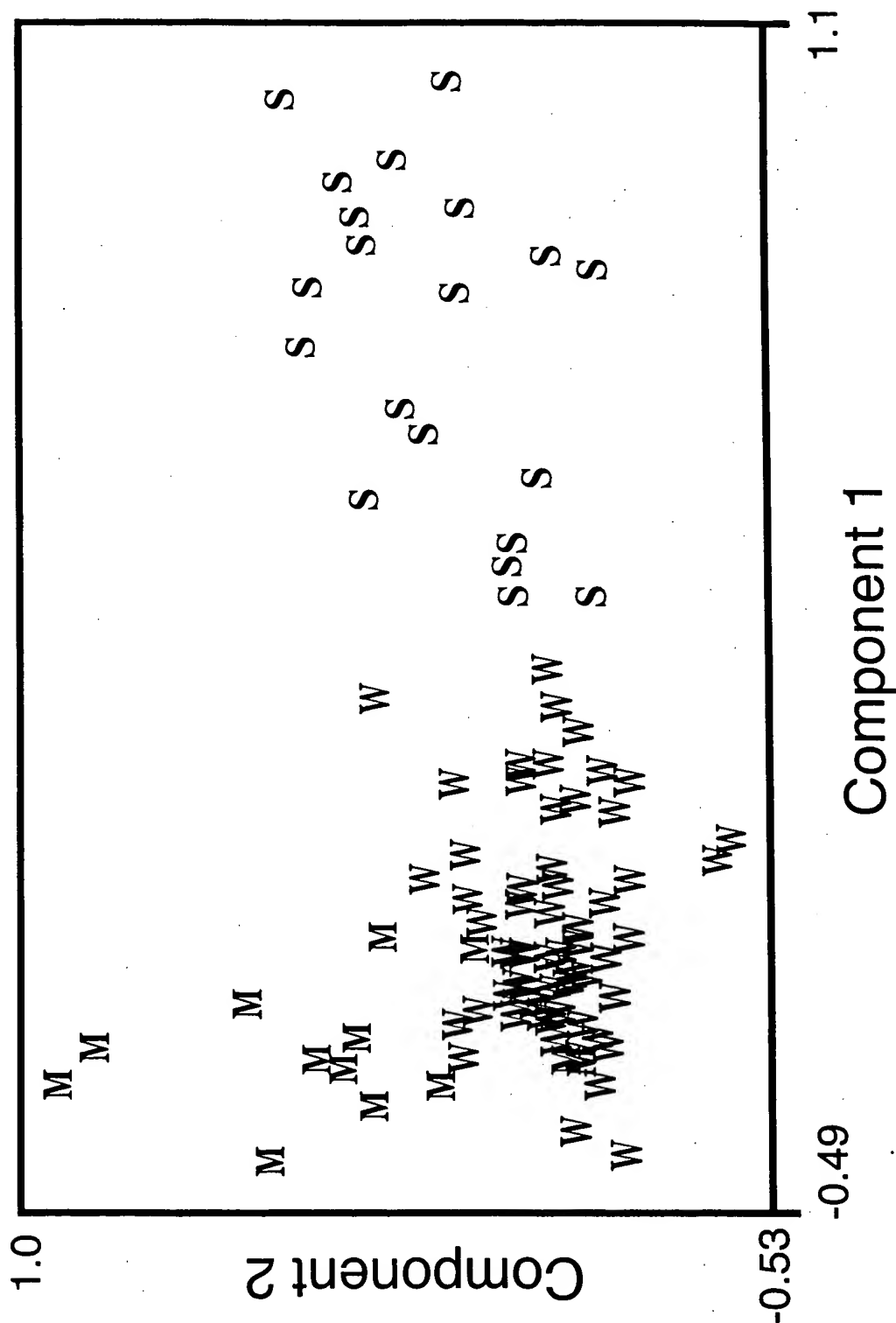


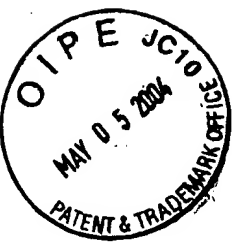
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FIG. 11



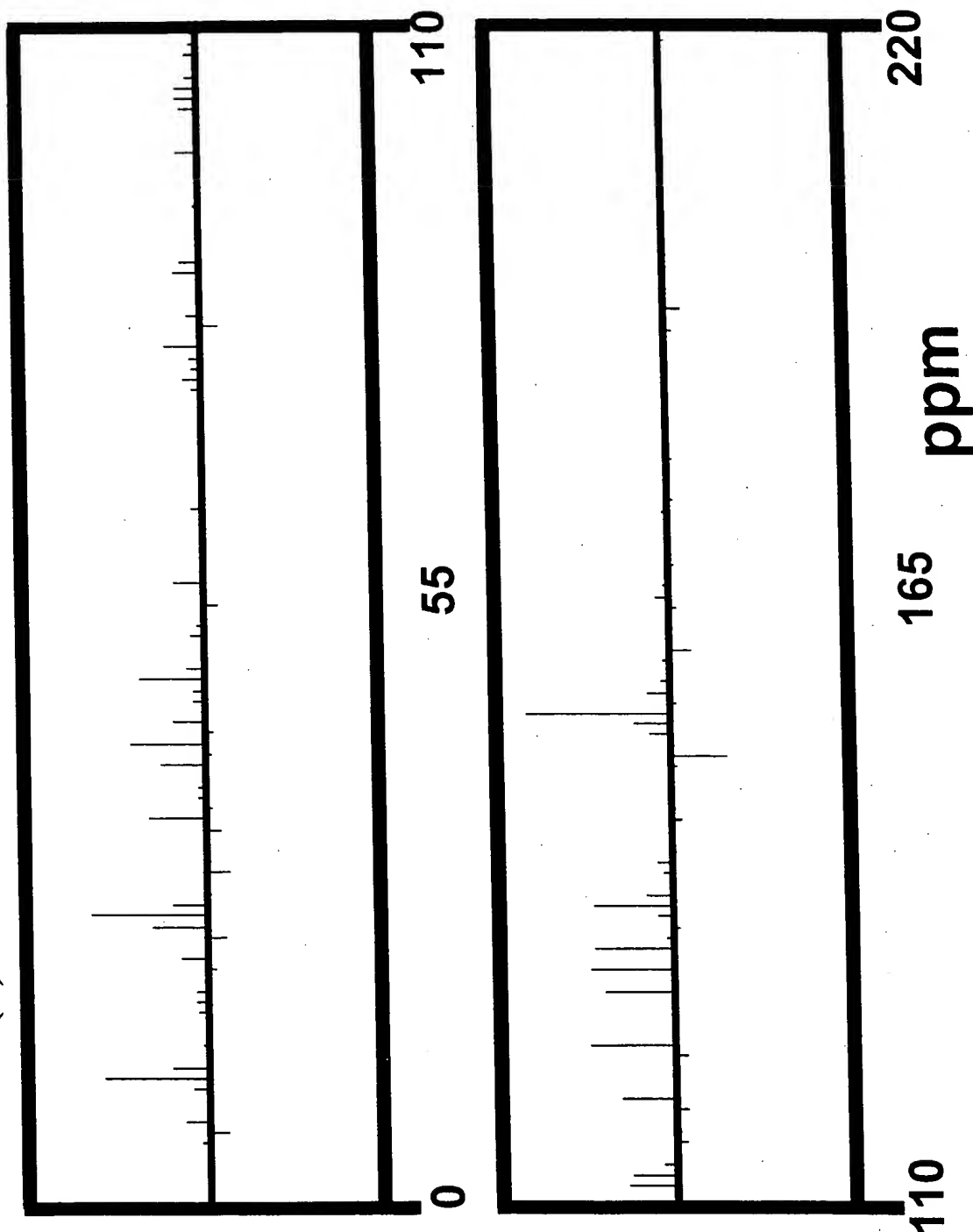


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FIG. 12(a)



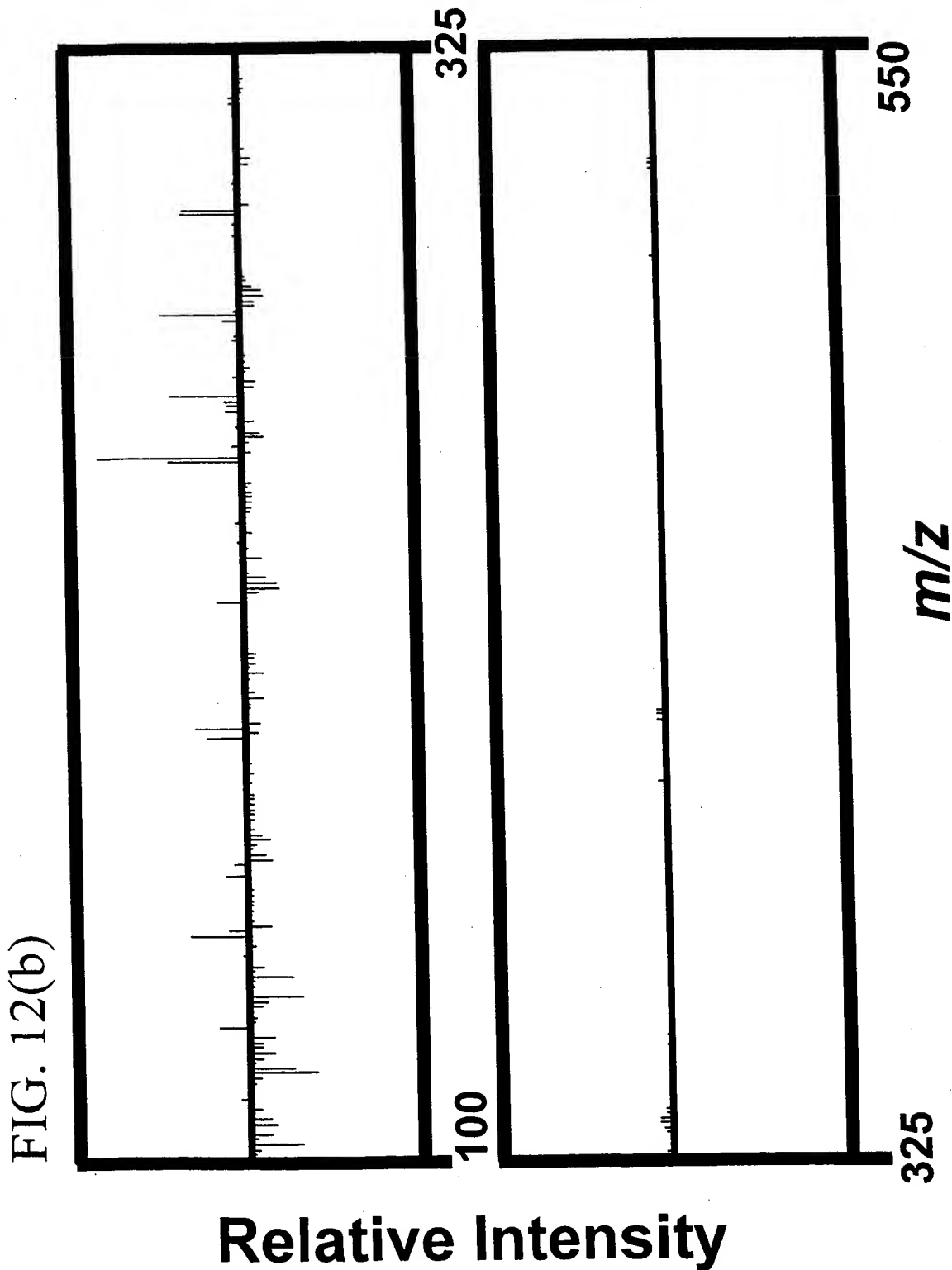
Relative Intensity



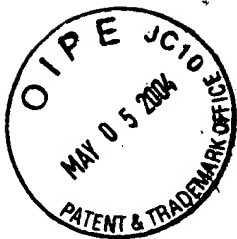
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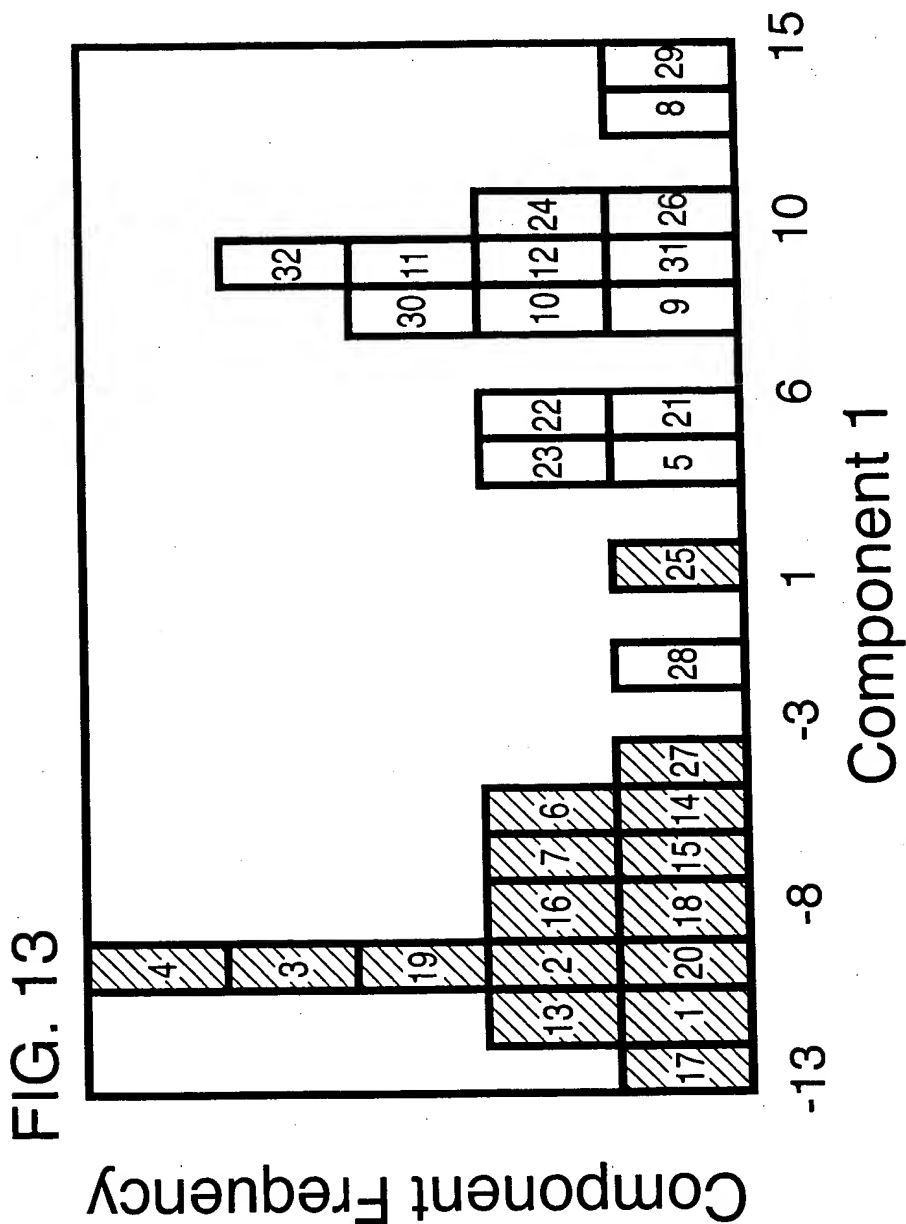
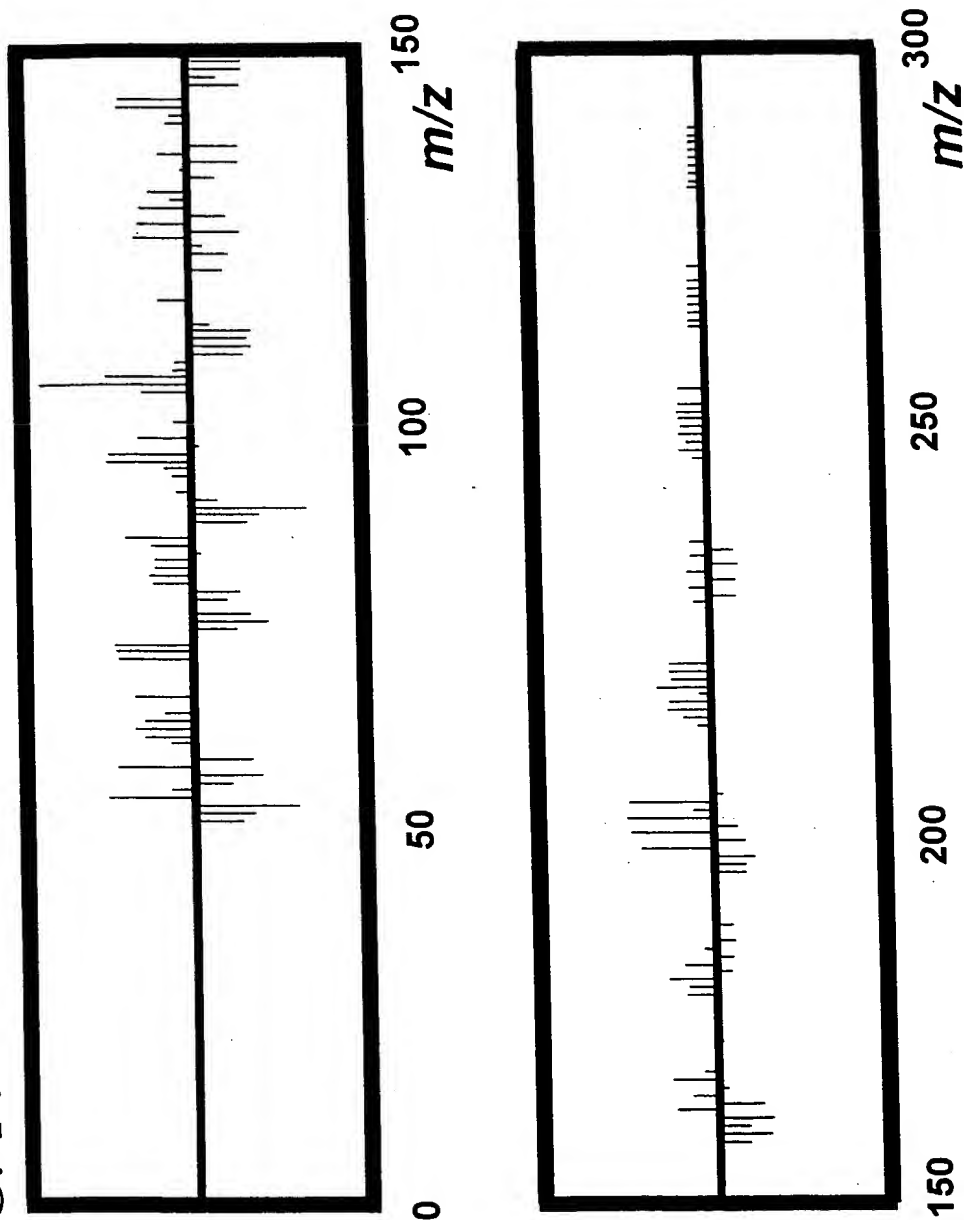
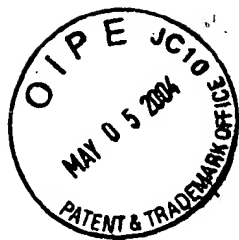


FIG. 14



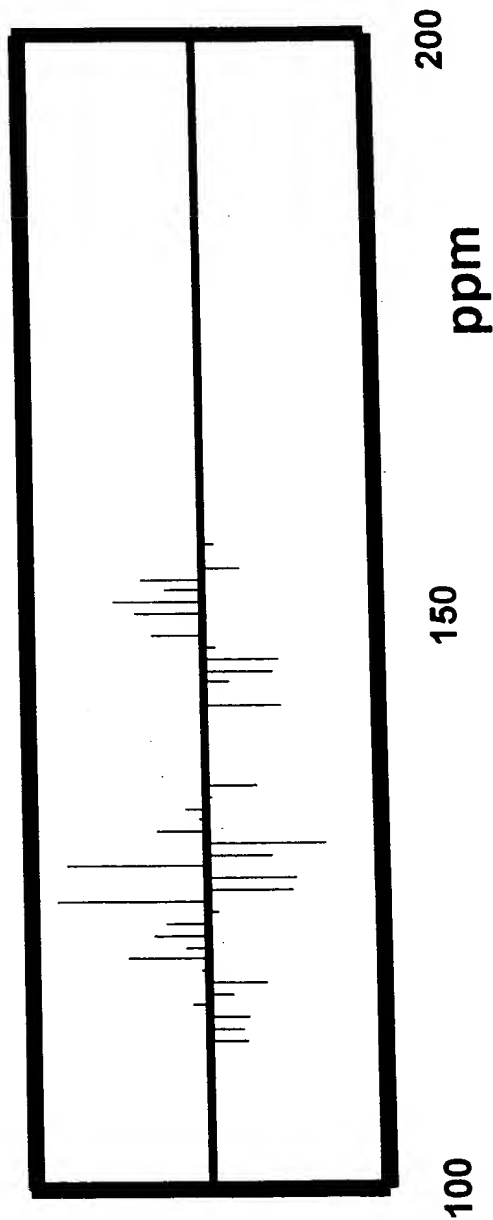


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FIG. 15



Relative Intensity

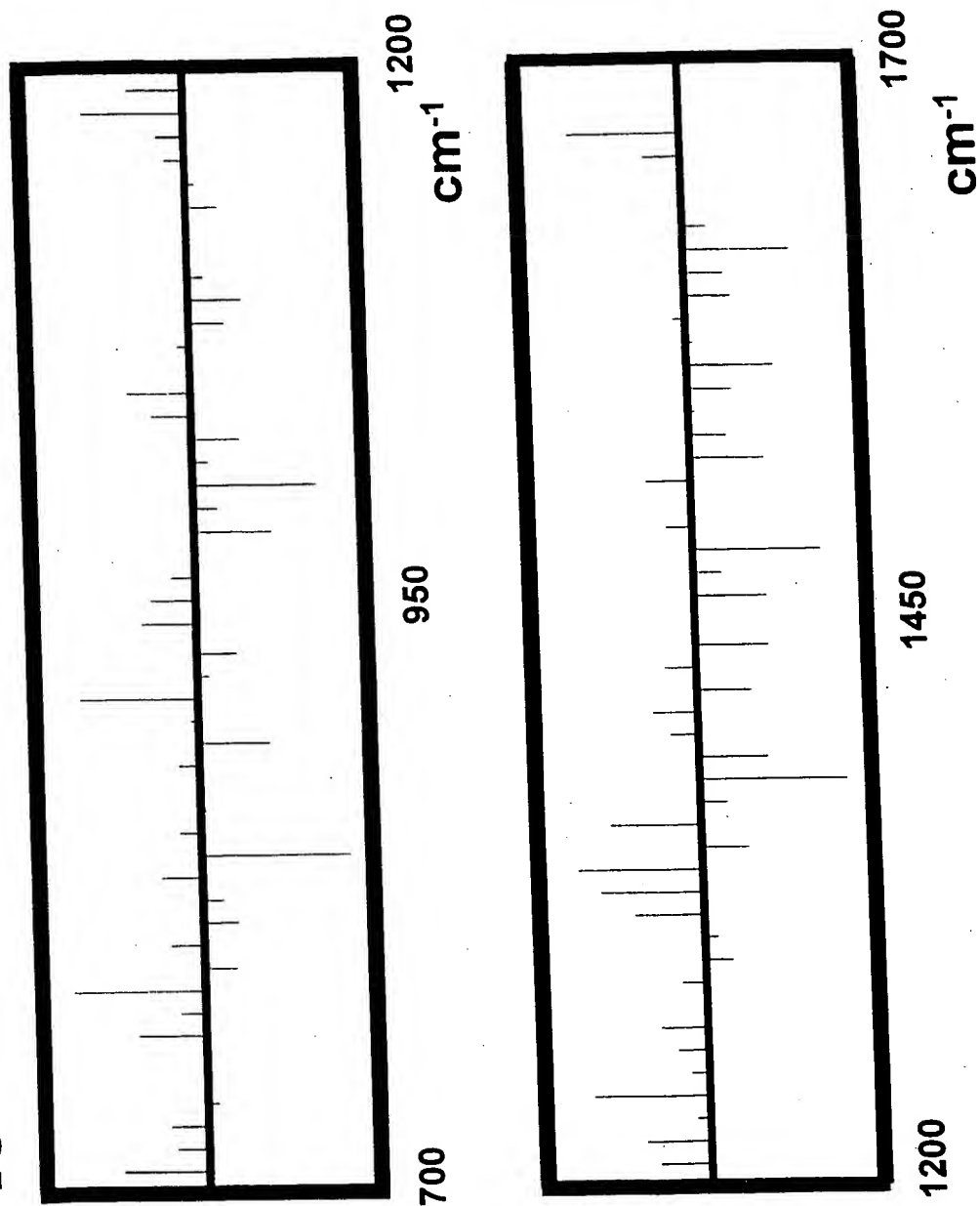


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FIG. 16



Relative Intensity

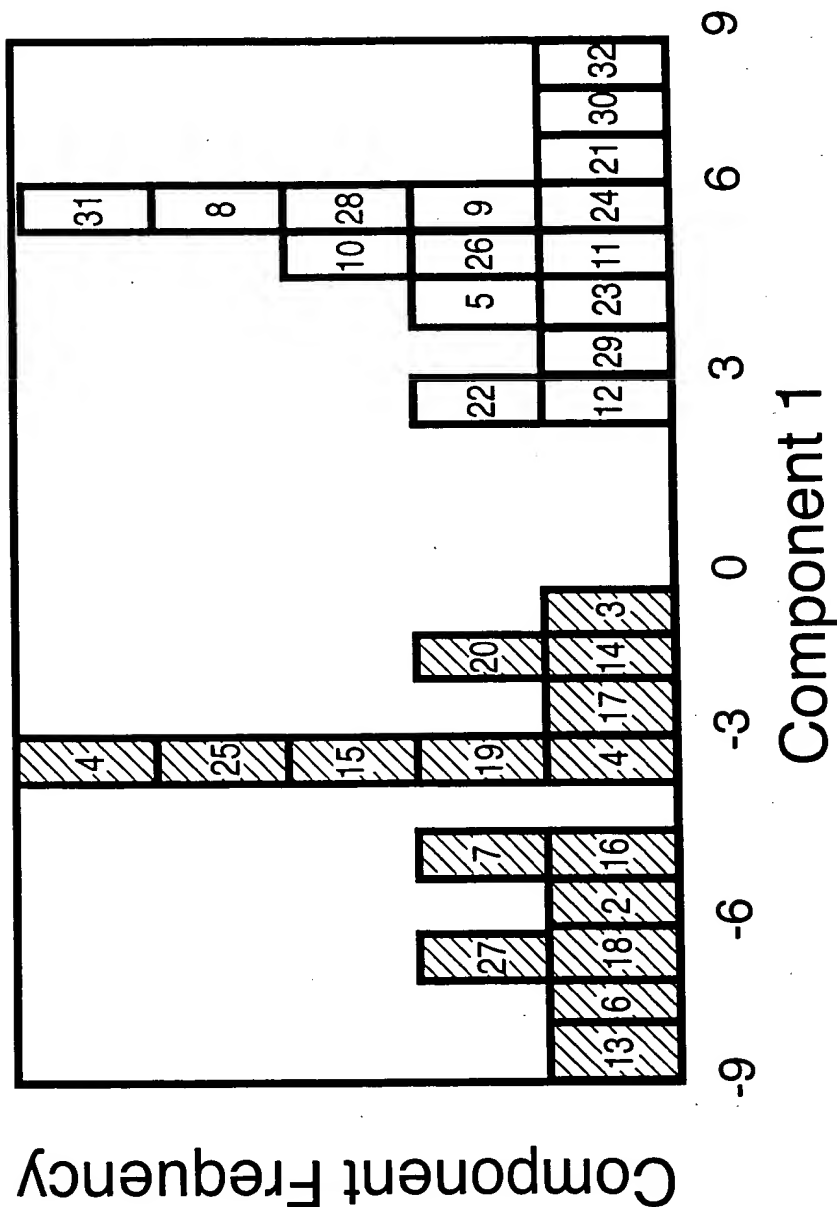


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FIG. 17



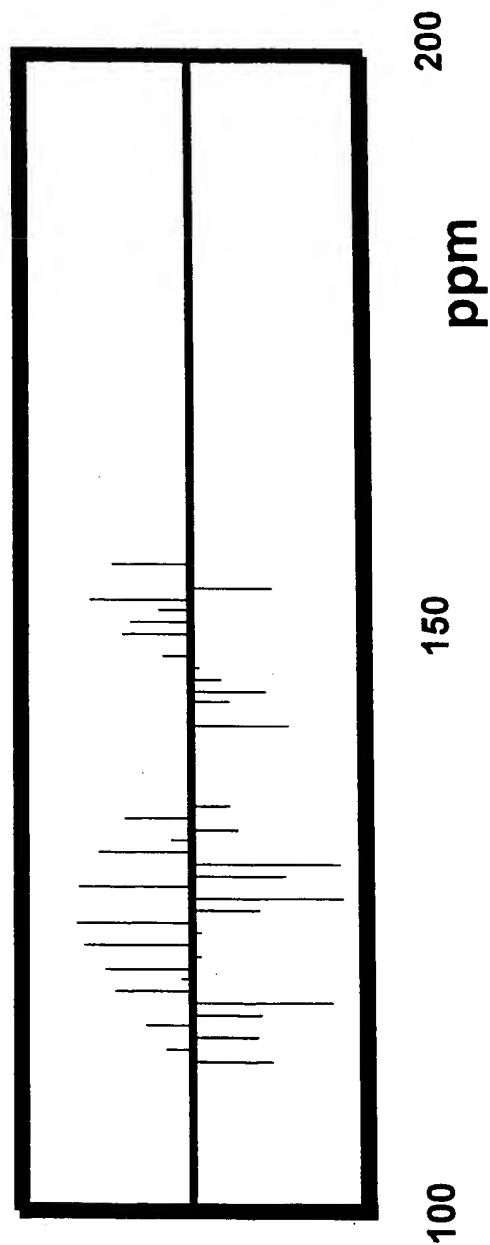


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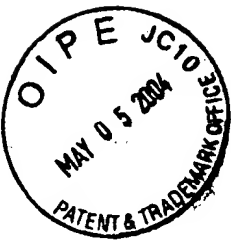
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FIG. 18



Relative Intensity

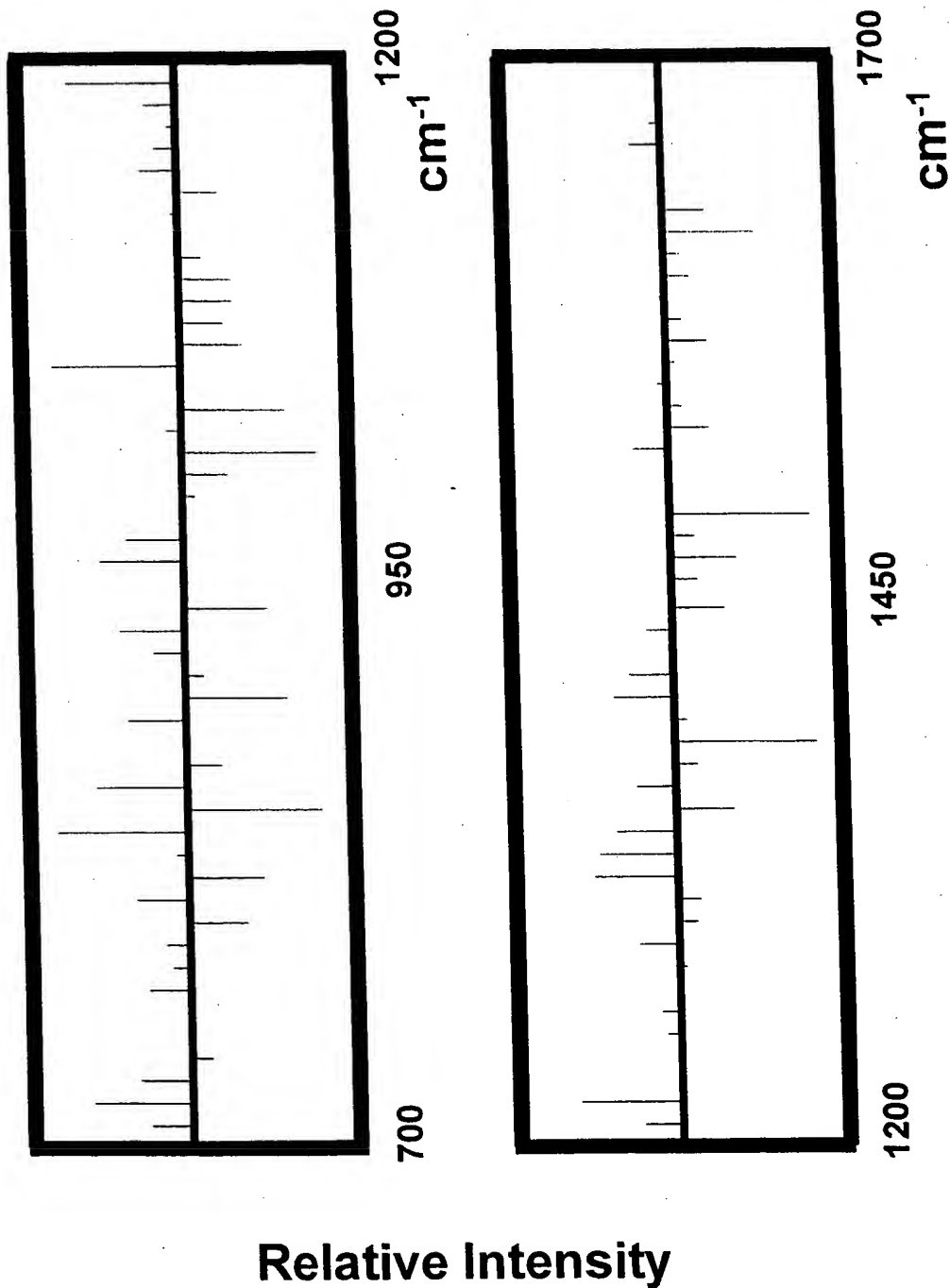


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Application No.: 09/629,557

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First Named Inventor: Miller et al.  
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FIG. 19



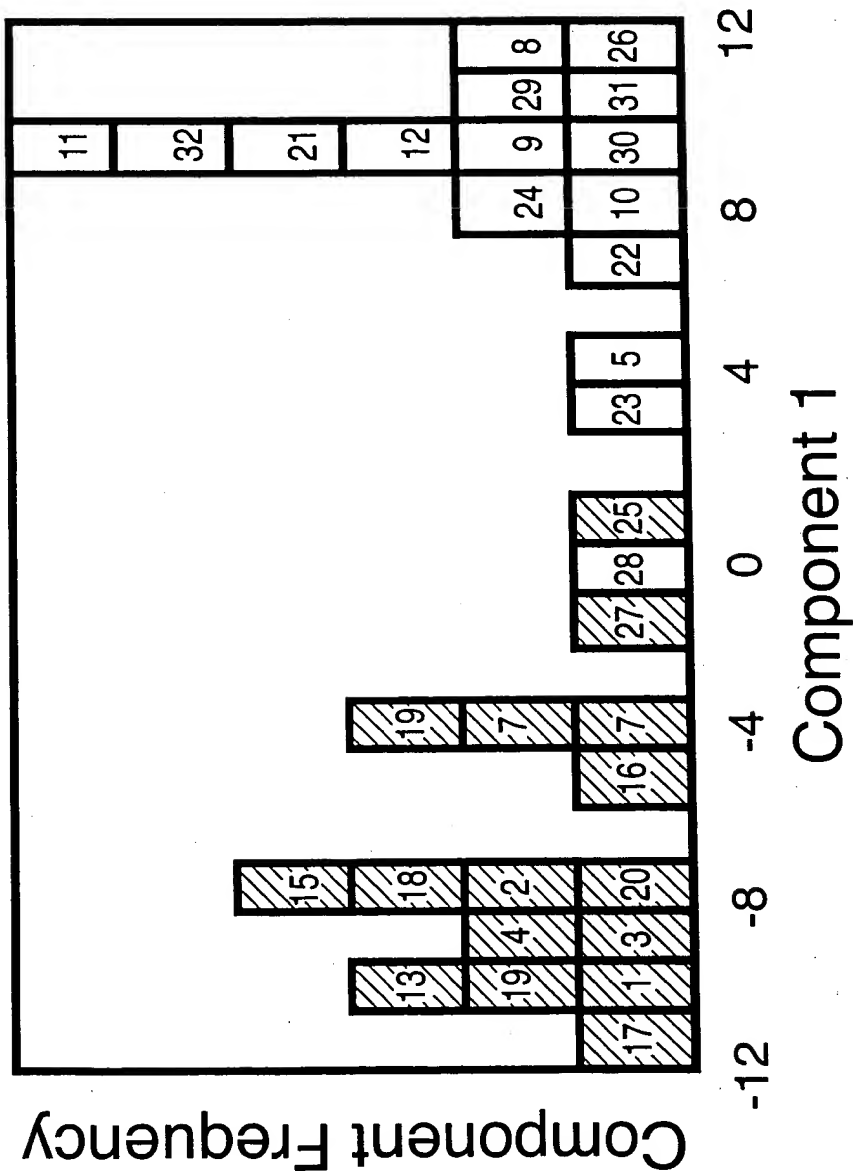


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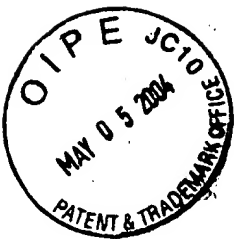
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FIG. 20





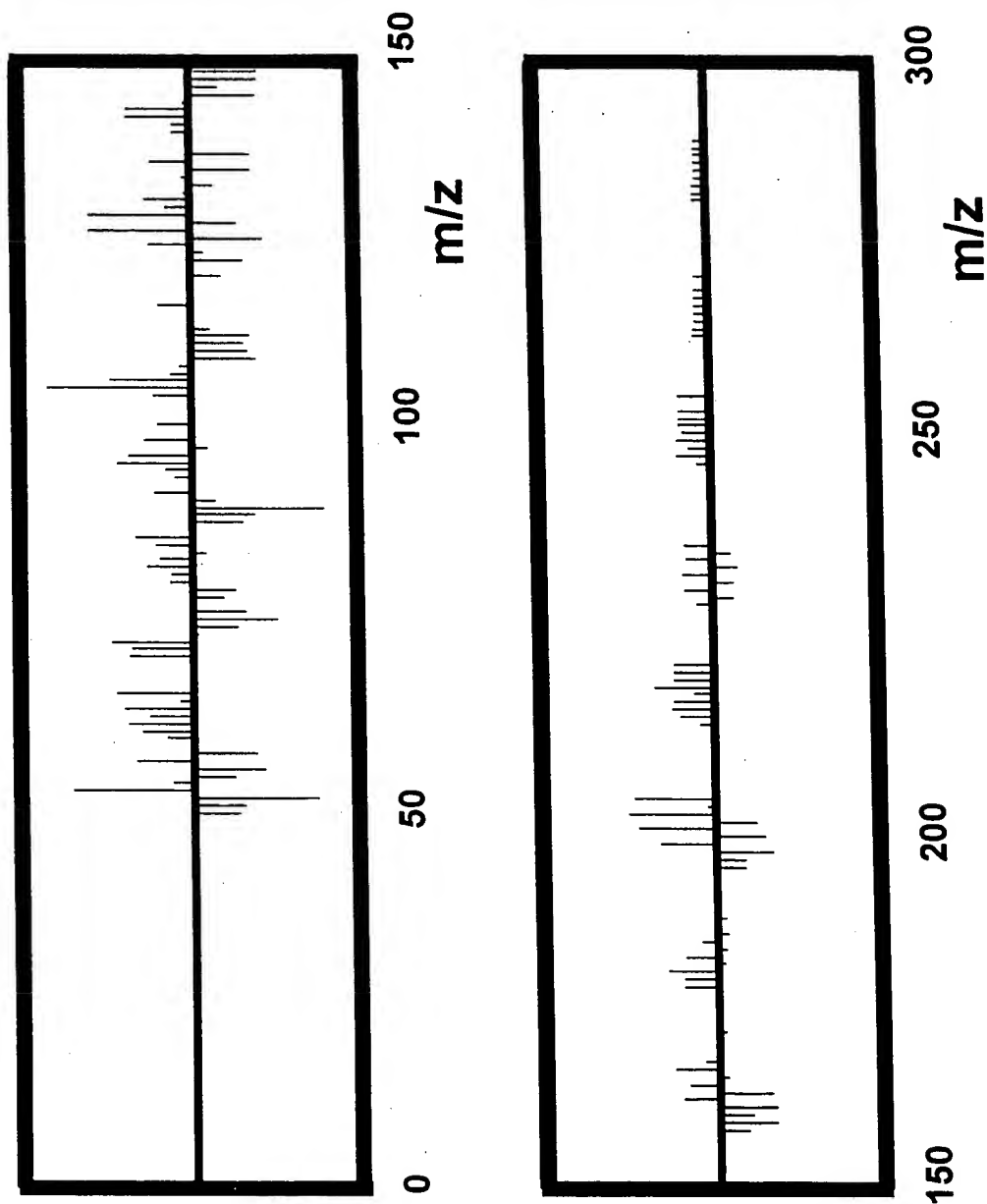


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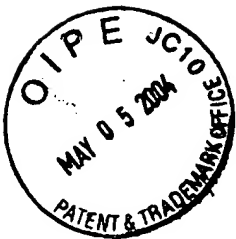
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FIG. 21



Relative Intensity

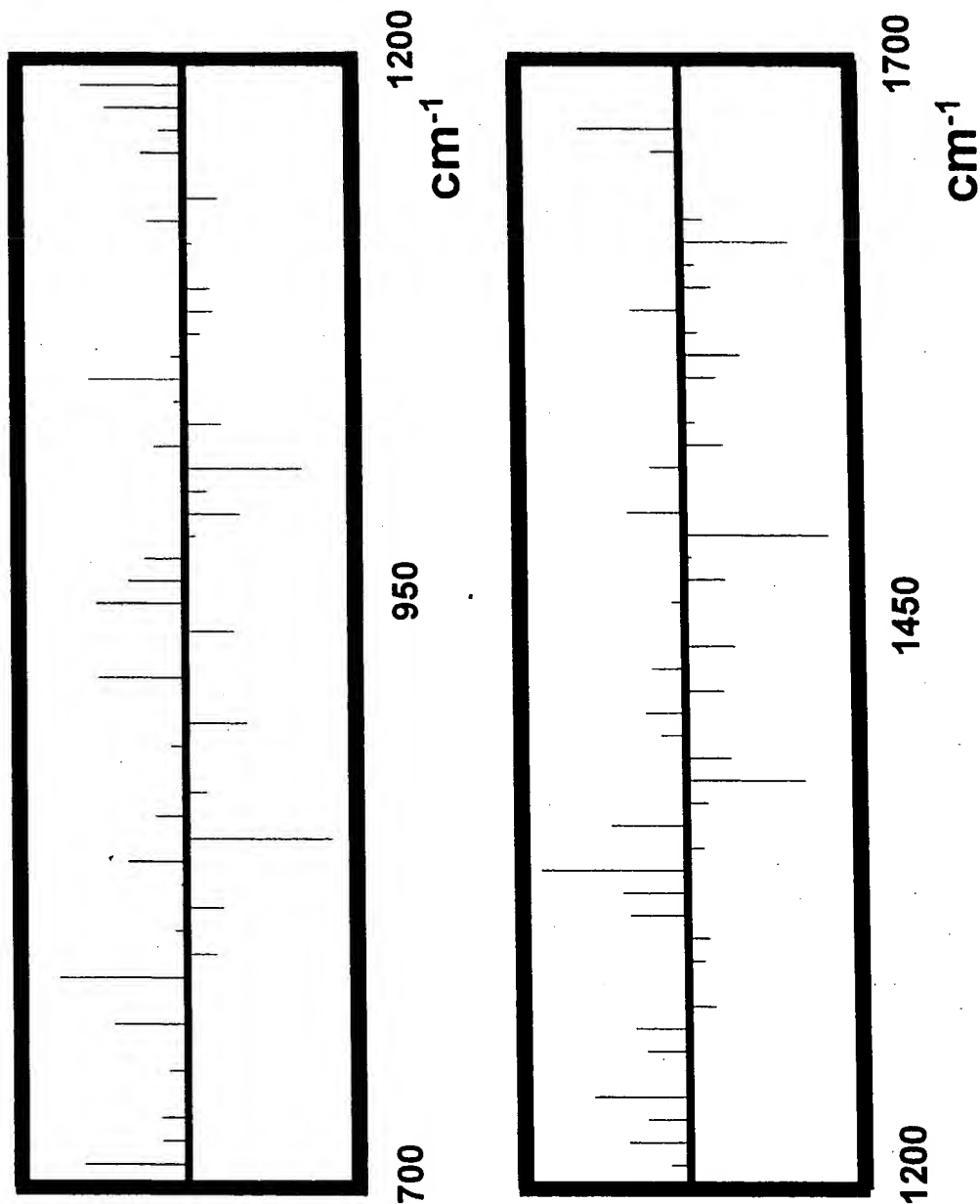


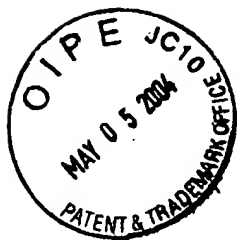
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FIG. 22



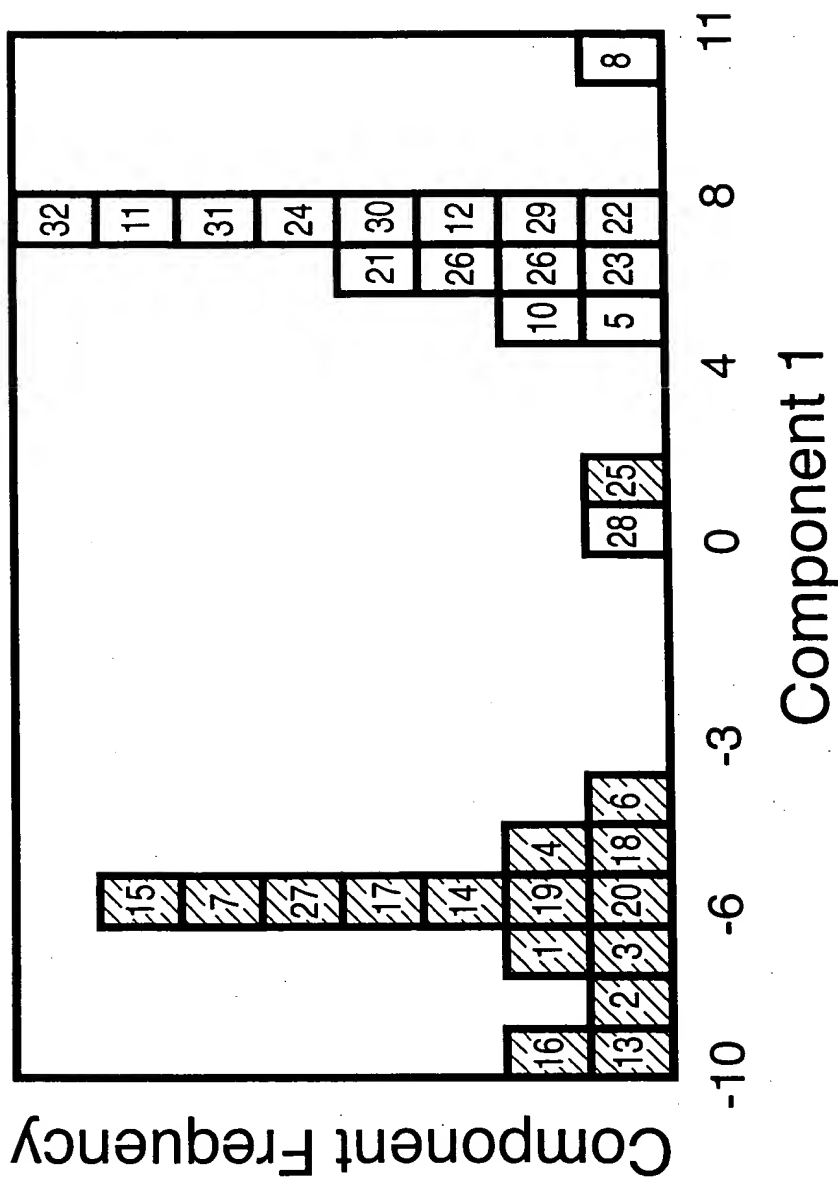


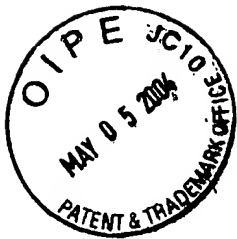
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FIG. 23



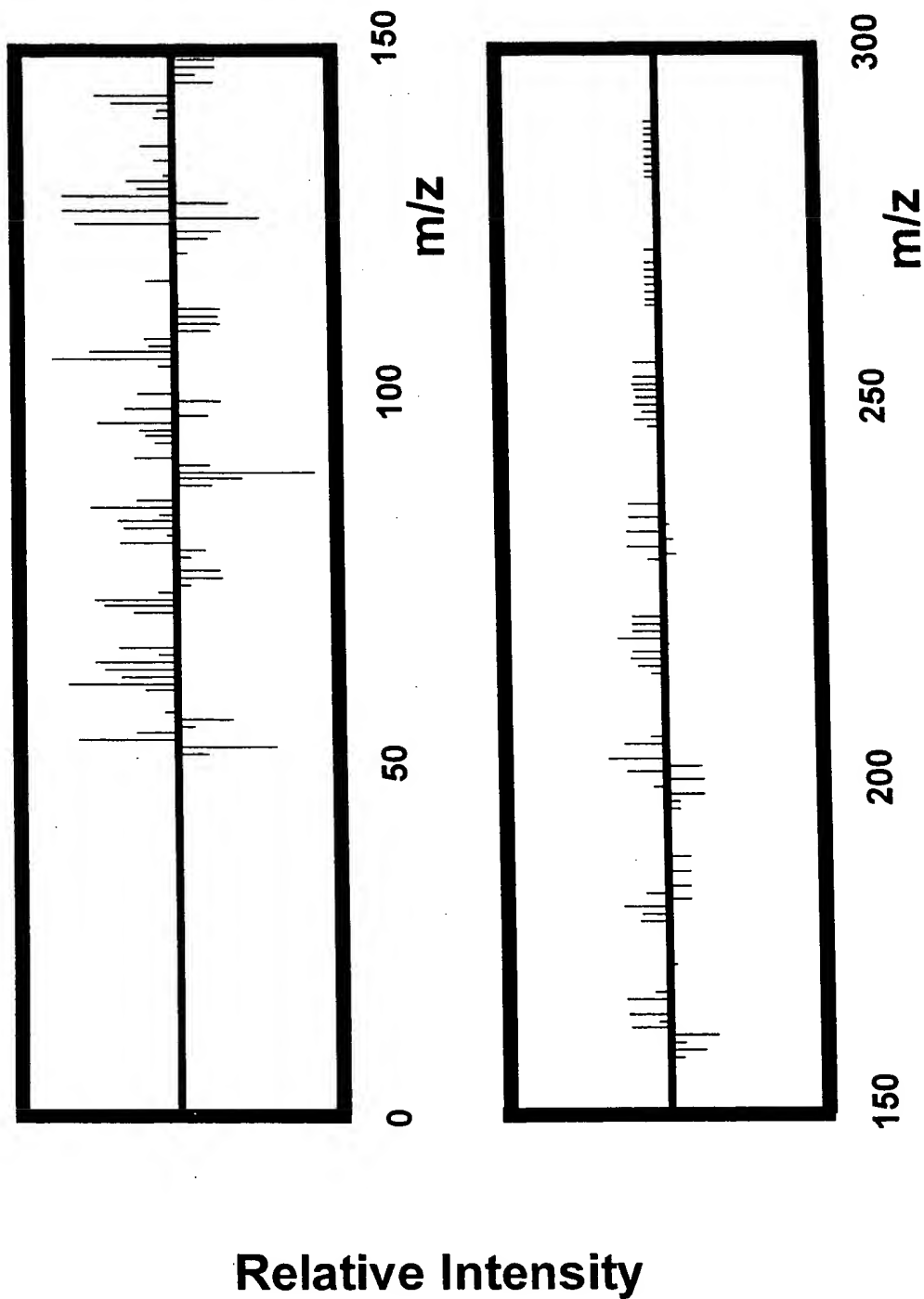


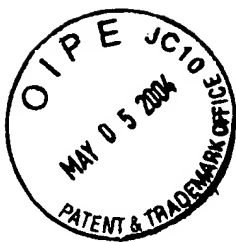
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FIG. 24



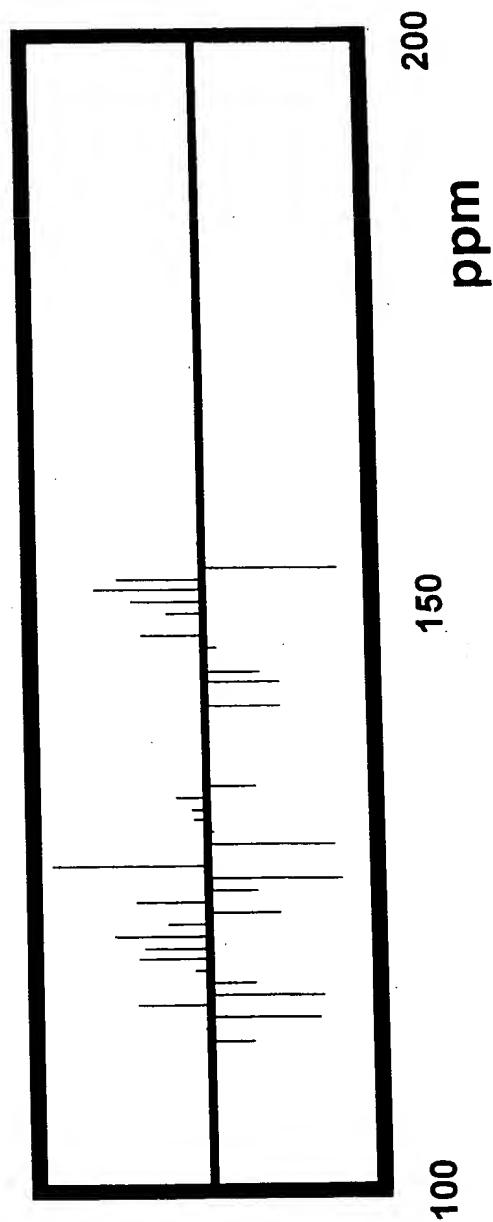


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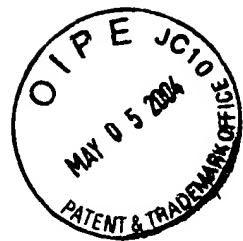
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FIG. 25



Relative Intensity



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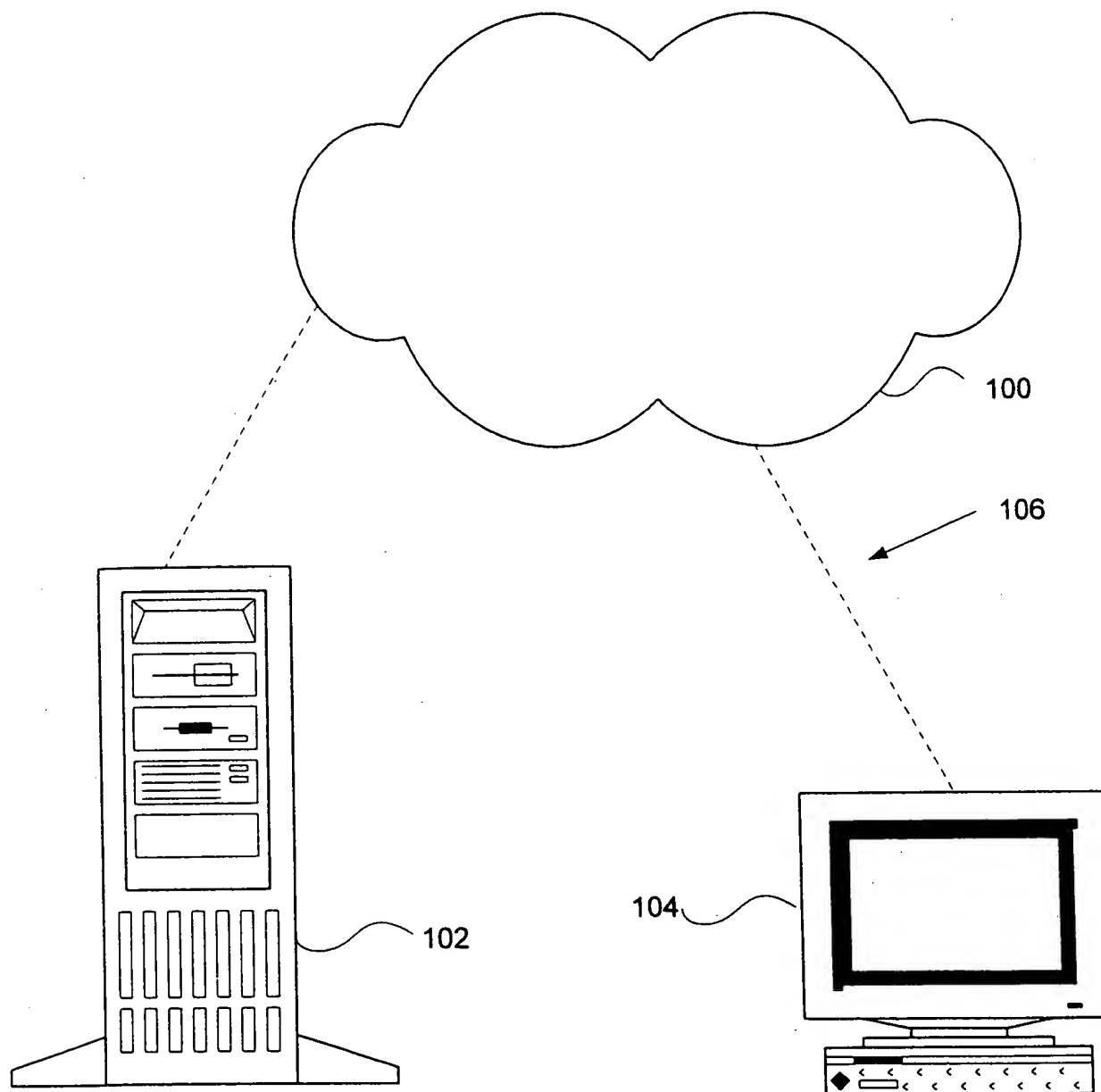
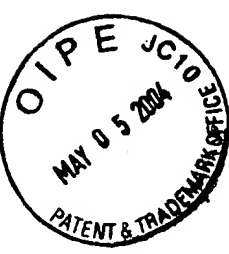


FIG. 26



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FIG. 27

